If only the CA coordinates of a model are deposited, nobody will ever be able to validate the model. Actually, in some cases this is possible nowadays.

One does not need to use non-crystallographic symmetry restraints. The examples to the contrary may make some want to re-do their most recent refinement (7).

Ramachandran plots are still stiflingly boring. On the contrary: they are extremely useful for model validation. We will show some highly entertaining examples from real-life models.

Considering the controversial nature of some aspects of this presentation, the audience is invited to disagree vehemently.

References:

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MS03.04.05 IMPROVED STRUCTURE REFINEMENT THROUGH MAXIMUM LIKELIHOOD. Randy J. Read and Navraj S. Pannu, Departments of Medical Microbiology & Immunology, and Mathematical Sciences, University of Alberta, Edmonton, Alberta T6G 2H7, Canada.

The least-squares target is not theoretically justified for crystal structure refinement, so it is preferable to use a maximum likelihood refinement method over least-squares for macromolecules. Maximum likelihood refinement has been implemented in the program REFMAC.

At each cycle the program performs two steps. First it estimates the overall parameters of likelihood. This is most successful when the parameters are deduced from the FreeR set of reflections. Secondly it uses these parameters to build the likelihood function and refine the atomic parameters.

At the end of a cycle REFMAC also writes weighted map coefficients to give less biased maps for rebuilding, taking care to restore the observed diffraction data. Absent reflections cause unpredictable noise in map calculations which may lead to errors in interpretation.

Several examples are described. In each case the refinement was carried over from an existing model. Results were compared to maps and phases generated from the final coordinates.

Different parts of structure may be assigned different expected errors and methods for doing this have been explored and implemented. Two important applications for this are being analysed. In the first case the structure contains several U atoms as well as protein atoms. In the second part of the structure has been interpreted from a poor RIR map but the other part is being modelled from the uninterpretable electron density. There is also an option to include available phase information, for example from MIR or MAD calculations.

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MS03.04.06 DESCRIPTION OF PROGRAM USING MAXIMUM LIKELIHOOD RESIDUAL FOR MACROMOLECULAR REFINEMENT, ILLUSTRATED BY SEVERAL EXAMPLES. Eleanor J. Dodson and Garib N. Murshudov, Chemistry Department, University of York, Heslington, York, U.K., and Alexei A. Vagin, UCMB-ULB, Free University of Brussels, Avenue Paul Heger 160/16 - P 1050 Brussels, Belgium.

We illustrate the advantages of the maximum likelihood refinement method over least-squares for macromolecules. Maximum likelihood refinement has been implemented in the program REFMAC.

At each cycle the program performs two steps. First it estimates the overall parameters of likelihood. This is most successful when the parameters are deduced from the FreeR set of reflections. Secondly it uses these parameters to build the likelihood function and refine the atomic parameters.

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Several examples are described. In each case the refinement was carried over from an existing model. Results were compared to maps and phases generated from the final coordinates.

Different parts of structure may be assigned different expected errors and methods for doing this have been explored and implemented. Two important applications for this are being analysed. In the first case the structure contains several U atoms as well as protein atoms. In the second part of the structure has been interpreted from a poor RIR map but the other part is being modelled from the uninterpretable electron density. There is also an option to include available phase information, for example from MIR or MAD calculations.